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Framework for Construction of Multi-scale Models for Biological Wastewater Treatment Processes - Case Study: Autotrophic Nitrogen Conversion

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Abstract
In wastewater treatment technologies, employing biofilms or granular biomass, processes might occur at very different spatial and temporal scales. Model development for such systems is typically a tedious, complicated, and time consuming task, which involves selecting appropriate model equations for the different scales, making appropriate and simplifying assumptions, connecting them through a defined linking scheme, analyzing and solving the model equations numerically, and performing parameter estimations if necessary. In this study, a structured framework for modeling such systems is developed. It aims to support the user at the various steps and to reduce the time it takes to generate a model ready for application. An implementation of the framework is illustrated using a simple case study, which considers treatment of a nitrogen-rich wastewater via nitritation.
Keywords
Modeling framework; multi-scale model; wastewater treatment; nitrogen conversion; AOB

Introduction

Models are playing an increasingly important role in design and optimization of wastewater treatment plants and processes. Models have successfully been used for many purposes, from design to supporting process operation and control of treatment plants, or as a tool to evaluate the performance of a specific treatment technology. An area which has been receiving decreased attention is the application of models as a tool for design of experiments when investigating new and emerging processes. By utilizing models for this purpose, the practical experiments can be more targeted towards a specific goal of the study or towards testing a specific hypothesis. As a consequence, it is expected that the number of experiments to be performed can be reduced, which will decrease the man power needs and the cost of process development. In addition, the effect of operational conditions can be explored and help direct practical experiments towards obtaining optimal process performance. For all the above mentioned purposes development of appropriate and reliable models are of great importance. A systematic framework generating models in an efficient and structured way has therefore been developed in this work. The framework is illustrated by a simple case study regarding biological oxidation of ammonium to nitrite performed by ammonium oxidizing bacteria (AOB).

Methods

In biofilm systems, processes happen at very different spatial scales, as opposed to in completely mixed reactors where all reactions are assumed to happen at the same spatial scale. Modeling biofilm systems typically involves three spatial scales (Xavier et al., 2005); individual cells, biofilm, and reactor scale, as shown in Figure 1. On the individual or cellular scale the growth and metabolism of the microorganisms are captured. On the biofilm scale the spatial location of the bacteria is described, and also the transport of soluble and particulate compounds is included here. At the reactor scale the overall mass balances are considered along with the hydrodynamic conditions in the reactor.

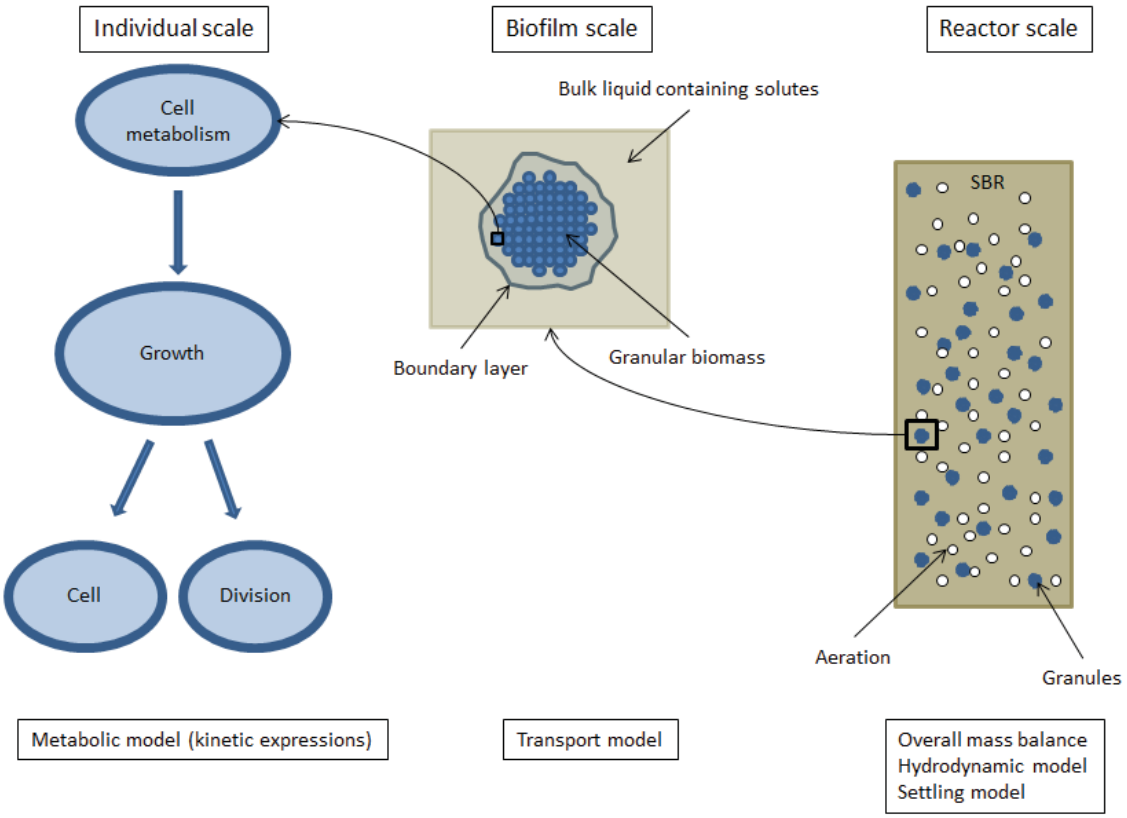

Figure 1. Conceptual model of an SBR with granular biomass, as an example of a multi-scale model. Three spatial scales are considered; the individual or cellular, biofilm, and reactor scale (adapted from Xavier et al., 2005).

At the cellular scale, individual cells, a subset of a functional group (e.g. specific species of AOB), or an entire functional group of microorganisms (e.g. AOB) can be modeled. If individuals are considered, a certain differentiation in their metabolism might be assumed, whereas if a subset or entire functional group is modeled, their metabolism can be assumed to be identical. The latter is termed the lumped approach and can be solved along with the transport equations at the biofilm scale.

A framework that supports the model construction at the different scales as well as linking them to each other has been developed, by studying the work flow typically involved in development of multi-scale systems (see Figure 2). The first step consists of defining the overall modeling objective. The second step is gathering system information such as for example physical and operational conditions of the system. From this information the main assumptions can be established in the third step. Subsequently, the model scenarios of interest should be defined, including which spatial scales and processes are of relevance. From this definition the individual models to be constructed can be derived. Each of the individual models are either taken from previous studies, if such exist, or they are constructed following the work flow depicted on the right side of Figure 2. First the specific model objective for the individual model and then the corresponding system information and assumptions are defined. The individual model is constructed, and sensitivity and identifiability analysis of the model parameters are conducted as necessary. The model is then calibrated to experimental data by adjusting the sensitive parameters. Finally, when the individual model has been validated, it is "exported" back into the multi-scale modeling work flow. The individual models are then linked to each other by defining the data needed to be transferred from one spatial scale to the next and vice versa. The multi-scale model system can now be solved by defining appropriate initial and boundary conditions.

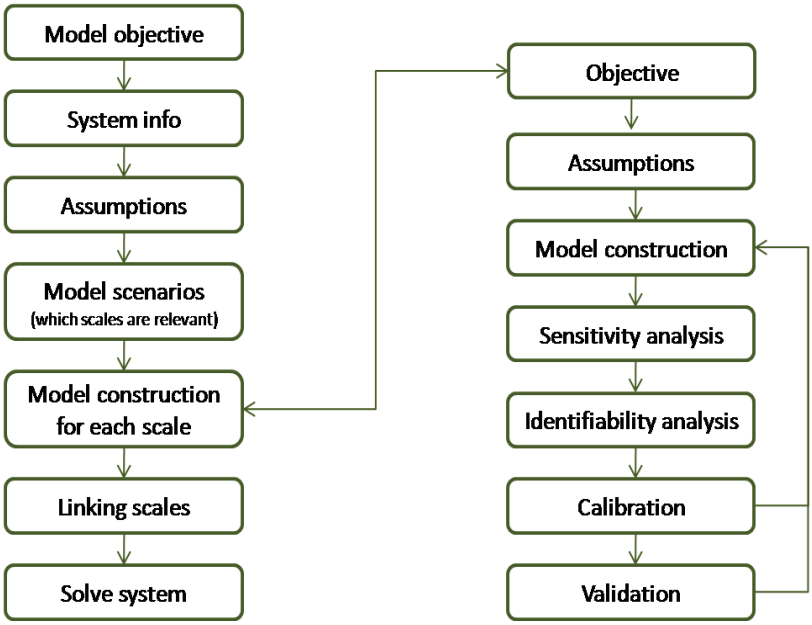

Figure 2. Work flow scheme for multi-scale modeling (left) and identification of the individual models (right) (adapted from Heitzig et al, 2010).

Case study. Nitritation, the process in which ammonium is biologically converted to nitrite, is the first step in the nitrification process and is also utilized in complete autotrophic nitrogen removal (CANR), which is a relatively new treatment technology. For wastewaters containing high concentrations of nitrogen and low organic carbon to nitrogen ratios, such as sludge digestion liquor, landfill leachate, or special industrial wastewaters, conventional nitrification-denitrification is either not a very efficient treatment process or a rather costly affair. CANR combining partial nitritation (eq. 1) with anaerobic ammonium oxidation (anammox) (eq. 2) can overcome these difficulties, because the requirement for aeration is lowered and the need for addition of organic carbon is eliminated (Strous et al., 1997). Meanwhile, the sludge production and the need for treatment of excess sludge are significantly lowered. The processes are performed by ammonium oxidizing bacteria (AOB) and anaerobic ammonium oxidizing bacteria (AnAOB), which require aerobic and anoxic conditions, respectively.

$$NH_4^+ + 1.5O_2 \rightarrow NO_2^- + H_2O + 2\ H^+ \quad (1)$$

$$NH_4^+ + 1.32\ NO_2^- + 0.066\ HCO_3^- + 0.13\ H^+ \rightarrow$$

$$0.26\ NO_3^- + 1.02\ N_2 + 0.066\ CH_2O_{0.5}N_{0.15} + 2.03\ H_2O \quad (2)$$

An environment where both groups of bacteria can co-exist can be created in biofilms or granular biomass, where both anoxic and aerobic conditions are created. In the outer layers AOB will grow, consume oxygen, and prevent oxygen from penetrating further than a certain depth. In the anoxic inner biofilm layers the AnAOB will be present.

In the case study the overall model objective is to study the growth of AOB and its metabolism (eq. 1) in a 1-dimensional flat biofilm. The biofilm surface area and reactor volume are both constant parameters with certain values (system info). No biomass is present in the bulk liquid, advective transport of soluble compounds is ignored, and all AOB are assumed to have a uniform metabolism (assumptions). The equations in the cellular and biofilm scale can thus be solved simultaneously. The model scenario considered therefore includes the biofilm and reactor scales. The individual models for the conversion and transport of soluble and particulate compounds can be seen in eq. 3 and 6, respectively. For the soluble compounds the biofilm scale is linked to the overall mass balance in the reactor scale (eq. 5) by the flux through the boundary layer between the biofilm and the bulk liquid (linking scales) (eq. 4).

$$\frac{\partial S_i}{\partial t} = -D_{i,biofilm}\frac{\partial^2 S_i}{\partial z^2} + r_i \quad (3)$$

r_i is the conversion rate and $D_{i,biofilm}$ is the diffusion coefficient of compound *i* in the biofilm.

$$j_{biofilm} = -D_{i,biofilm}\left(\frac{dS_i}{dz}(z = L_-)\right) = -k_c\left(S_{i,bulk} - S_{i,L_+}\right) \quad (4)$$

k_c is the mass transfer coefficient of compound *i* through the boundary layer, and $S_{i,L+}$ is the concentration of compound *i* at the biofilm/bulk interface.

$$\frac{\partial S_{i,bulk}}{\partial t} = \frac{Q\left(S_{i,bulk,in} - S_{i,bulk}\right) - j_{biofilm}A_{biofilm}}{V_{reactor}} \quad (5)$$

Q is the flowrate through the reactor, $A_{biofilm}$ is the surface area of the biofilm, $V_{reactor}$ is the volume of the entire reactor, and $S_{i,bulk,in}$ is the influent concentration.

The particulates are assumed to only be present in the biofilm and are therefore only modeled in the cellular and biofilm scale as:

$$\frac{\partial X_{AOB}}{\partial t} = -u_F\frac{\partial X_{AOB}}{\partial z} - X_{AOB}\frac{\partial u_F}{\partial z} + r_{AOB} \quad (6)$$

u_F is the biofilm growth velocity and r_{AOB} includes both the biomass growth and decay rates.

Results

A generic multi-scale modeling framework was implemented in the ICAS-MoT software (Heitzig et al., 2010), and is customized for the needs of biofilm systems by adapting the features of the software according to the work flow identified for multi-scale biofilm modeling, as shown in Figure 2. An appropriate multi-scale model for the case study is first generated using the software and following the structured steps in Figure 2 (i.e. numerical analysis (incidence matrix), optimal solution, sensitivity analysis, parameter estimation, etc). Then the constructed model is transferred to Matlab Simulink in appropriate form (the model can be exported as an object file, or exported as an m-file script implementation). The purpose here is to use the better capabilities of the Matlab Simulink environment to configure operational conditions and run different experiments in the case study. While the simple case is used to highlight the framework and the software support for multi-scale model development, more detailed and complex model systems, including more microbial species and higher numbers of soluble compounds, can easily be constructed in the future.

Conclusions

A framework for construction of multi-scale models of biofilms used in biological wastewater treatment processes has been constructed. The framework is implemented in the ICAS-MoT software, which guides and supports the user at different steps of the modeling process. It is flexible and efficient, which allows for generation of customized models for a broad range of applications from design of experiments for new processes to process design and optimization.

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